Bisphenol B

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 766 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

Image not found
Imazalil
Measured: 5370
Predicted: 264

Image not found
Pendimethalin
Measured: 5010
Predicted: 4980

Image not found
Isopropylpropyzamide
Measured: 148
Predicted: 173

Image not found
Siduron
Measured: 204
Predicted: 210

Image not found
N-Cycloheptyl-N'-phenylurea
Measured: 234
Predicted: 218